Seq No	Term	Variable	Description	Cat1|Cat2|...	freq
1	CHARMM DCD Trajectory File	.dcd	A widely used binary trajectory file format originating from CHARMM.	data format	2
2	Action	Action	A command that performs an operation on coordinate frames.	method|process	58
3	B-factor	bfactor	A value representing the thermal motion of atoms in a crystal structure.	measure	23
4	Cartesian Covariance Matrix	covariance	A matrix representing the covariance of atomic Cartesian coordinate fluctuations.	measure|data format	47
5	Connolly Surface	molsurf	An action to calculate the Connolly solvent-accessible or solvent-excluded surface area.	method|measure	7
6	Coordinate Translation	trans | translate	An action to translate specified atoms by a given vector.	method|process	1
7	correlation	corr	An analysis command to calculate auto- or cross-correlation of data sets.	analysis|method	108
8	Covariance Matrix	matrix	Calculates the covariance matrix of atomic fluctuations.	method|measure	186
9	constant pH simulation	cphstats	A simulation technique that allows protonation states of residues to change.	method|process	8
10	atomic positional fluctuations	crdfluct	A measure of the mobility of individual atoms in a simulation.	measure	7
11	Dihedral covariance matrix	dihcovar	A covariance matrix constructed from the dihedral angles of a molecule.	measure|model	12
12	distance RMSD	dme	RMSD calculated from a matrix of internal distances, not coordinates.	measure	9
13	Potential Energy	energy	Calculates potential energy terms (bond, angle, nonbonded, etc.).	measure|method	133
14	Potential Energy Calculation	energy	Calculates potential energy components for a molecular system.	method|measure	133
15	Ensemble Trajectory Processing	ensemble	Processes a set of trajectories as a synchronized ensemble.	method|process	55
16	Grid Inhomogeneous Solvation Theory	gist	An analysis method to map solvent structure and thermodynamics.	method|algorithm	102
17	Grid Binning	grid	An action that bins atomic positions onto a three-dimensional grid.	method|process	152
18	Hydrogen Bond Analysis	hbond	An action to identify hydrogen bonds based on geometric criteria.	method|analysis	32
19	Isotropically Distributed Ensemble Analysis	idea	An analysis method for characterizing internal protein dynamics.	method|analysis	19
20	Periodic Boundary Imaging	image	An action that wraps coordinates back into the primary periodic box.	method|process	54
21	trapezoid integration	integrate	A numerical method to approximate a definite integral using trapezoids.	algorithm	6
22	Isotropic Reorientational Eigenmode Dynamics	ired	An analysis method to study molecular reorientational motions.	method|analysis	60
23	J-Coupling	jcoupling	Calculates scalar coupling constants from dihedral angles.	measure|method	11
24	kcal/mol	kcal/mol	A unit of energy commonly used in molecular simulations.	unit	16
25	kernel density estimator	kde	A non-parametric method to estimate the probability density function of a variable.	algorithm|model	12
26	Kullback-Leibler divergence	divergence	A measure of how one probability distribution is different from a second.	measure|analysis	11

27	LCPO Surface Area	surf	An action to calculate solvent accessible surface area using the LCPO algorithm.	measure|method	12
28	LES Trajectory Splitting	lessplit	An action to split or average frames from Locally-Enhanced Sampling trajectories.	method|process	3
29	Linear Interaction Energy	lie	An action to calculate non-bonded interaction energy between a ligand and its surroundings.	method|measure	6
30	lifetime curve	curveout	A plot showing the survival probability of a state over time.	measure|analysis	10
31	Lipid Order Parameter	lipidorder	Calculates the deuterium order parameter (SCD) for lipid acyl chains.	measure|method	4
32	Structure Modification	makestructure	Modifies a structure by setting specified dihedral angles to new values.	method|process	9
33	asymmetric unit	mask	The smallest part of a crystal from which the whole is generated.	model|chemical entity	517
34	Maxwell-Boltzmann Distribution	Maxwellian distribution	A probability distribution for the speeds of particles at a given temperature.	model	2
35	two-state transition	meltcurve	A model where a system exists in only two distinct states (e.g., folded/unfolded).	model	3
36	Boltzmann statistics	modes	Classical statistics used to populate vibrational modes at high temperatures.	model	38
37	MPI (Message Passing Interface)	MPI	A standardized message-passing system for parallel computing.	software|method	46
38	Mean Square Displacement	MSD	A measure of the average distance a particle travels.	measure	45
39	NetCDF	NetCDF	A set of software libraries and self-describing, machine-independent data formats.	data format	16
40	Nuclear Overhauser Effect	NOE	The transfer of nuclear spin polarization from one nucleus to another.	measure|method	39
41	Nucleic Acid Structure Analysis	nastruct	An action to calculate a comprehensive set of nucleic acid parameters.	method|analysis	14
42	OpenMP	OpenMP	A parallel programming model for shared-memory multiprocessing.	software|method	28
43	In-Queue Trajectory Output	outtraj	An action to write a trajectory frame within the action queue.	method|process	20
44	Pair Distribution Function	pairdist	Describes the probability of finding a particle at a distance from another.	measure|method	18
45	Pairwise Energy	pairwise	Calculates pairwise non-bonded interaction energies between selections.	measure|method	33
46	Per-Residue RMSD	perres	An option to calculate the no-fit RMSD for each residue individually.	measure|method	20
47	Picosecond	ps	A unit of time equal to 10^-12 seconds.	unit	21
48	Principal Axes	principal	Calculates the principal axes of inertia for a selection of atoms.	measure|method	25
49	Coordinate Projection	projection	Projects trajectory coordinates onto eigenvectors (e.g., from PCA).	method|process	24
50	Sugar Pucker	pucker	Describes the 3D conformation of a sugar ring.	measure|chemical entity	72
51	quaternion RMSD	qrmsd	A computationally efficient method for calculating RMSD using quaternions.	algorithm|measure	6
52	Radial Distribution Function	radial	Describes how density varies as a function of distance.	method|measure	9
53	Radius of Gyration	radgyr | rog	An action to calculate the radius of gyration for a selection.	method|measure	11
54	Ion Randomization	randomizeions	Randomly swaps the positions of specified ions and solvent molecules.	method|process	4
55	Reference Structure	reference	A single coordinate frame used for alignment or comparison.	data source|state	381

56	linear regression	regress	A statistical method to model the relationship between a dependent and independent variable.	algorithm|method	14
57	Cell Replication	replicatecell	Creates a supercell by replicating the unit cell in specified directions.	method|process	5
58	rotational diffusion	rotdif	The process by which molecules reorient due to random rotational motion.	process|measure	18
59	Restraint	rst	A potential energy term used to restrict molecular geometry.	model|method	11
60	running average	runningavg	An average calculated over a sliding window of consecutive data points.	measure|analysis	14
61	Coordinate Scaling	scale	Scales the coordinates of selected atoms by specified factors.	method|process	31
62	SHAKE	SHAKE	A constraint algorithm used to fix bond lengths in simulations.	algorithm|method	15
63	SPAM (Spatial Properties of Activity by Mapping)	spam	An action to estimate relative free energies of hydration-shell waters.	method|algorithm	19
64	stfcdiffusion	stfcdiffusion	A command to calculate diffusion using a specific routine from STFC.	method|analysis	4
65	strip	strip	A command to remove specified atoms from the system and topology.	process	41
66	Symmetry-Corrected RMSD	symmrmsd	An action to calculate RMSD considering molecular symmetry.	measure|method	10
67	System Temperature Calculation	temperature	An action to calculate the system temperature from atomic velocities.	measure|method	51
68	DV/DL	ti	The derivative of the potential energy with respect to the coupling parameter lambda.	measure	25
69	Frame Time Modification	time	An action to add, remove, or modify time information in frames.	method|process	218
70	spherical harmonics	timecorr	A set of orthogonal functions on the surface of a sphere used in vector correlation.	model|algorithm	12
71	Toroidal Diffusion	tordiff	An action to calculate diffusion using a toroidal-view-preserving scheme.	measure|method	6
72	unstrip	unstrip	A command to undo a 'strip' operation, restoring original topology.	process	7
73	unwrap	unwrap	A command to make molecular trajectories continuous across periodic boundaries.	process|method	30
74	eigenvector	vecs	A non-zero vector that changes at most by a scalar factor when a linear transformation is applied.	measure|model	27
75	vector	vector	A command to define and track vector quantities over a trajectory.	analysis|measure	122
76	Velocity Assignment	setvelocity	Assigns atomic velocities from a Maxwell-Boltzmann distribution at a given temperature.	method|process	3
77	Velocity Autocorrelation Function	VAC	A function describing the correlation of a particle's velocity over time.	measure|analysis	10
78	Unit Cell Volume	volume	An action to calculate the volume of the periodic unit cell.	measure|method	20
79	Volumetric Map	volmap	An action to create a 3D density map of atomic positions.	method|process	12
80	watershell	watershell	A command to count solvent molecules within specified distances of a solute.	method|analysis	5
81	xtalsymm	xtalsymm	A command to handle crystal symmetry operations for superimposing subunits.	method|process	4
82	Cpptraj	Cpptraj	A program for processing molecular dynamics trajectories and data.	software	243
83	ptraj	ptraj	The predecessor program to cpptraj for trajectory analysis.	software	18
84	Topology	topology	Describes molecular connectivity, atom types, and parameters.	data format|model	263
85	Xmgrace Format	.agr	A data file format for the Grace plotting tool.	data format	5

86	Root-Mean-Square Deviation	rmsd	A measure of the average distance between atoms.	measure|method	117
87	Closest Action	closest	An action to find atoms within a certain distance.	method|process	24
88	Stripped Topology File	stripped topology file	A topology file corresponding to a structure after atom removal.	data format	2
89	Interactive Mode	interactive mode	A command-line shell mode for running cpptraj commands sequentially.	method|state	10
90	Batch Mode	batch mode	A mode for executing a pre-written script of cpptraj commands.	method|state	2
91	Parameter/Topology File Keyword	parm	Keyword used to specify a topology (parameter) file.	identifier	171
92	Queued Command	Queued commands	Commands that are set up but executed later.	method|state	2
93	Immediate Command	Immediate commands	Commands that are executed as soon as they are encountered.	method|state	1
94	Analysis	Analysis	A command that processes data generated from actions or files.	method|process	115
95	Trajectory Processing Run	Run	The main execution process of reading frames and applying actions.	process	99
96	Ensemble Processing	ensemble processing	Simultaneously processing corresponding frames from multiple trajectories.	method|process	3
97	CUDA (Compute Unified Device Architecture)	CUDA	A parallel computing platform and API for NVIDIA GPUs.	software|method	19
98	Across-Trajectory Parallelism	across-trajectory parallelism	MPI strategy where trajectory frames are divided among processes.	method|algorithm	4
99	2D Root-Mean-Square Deviation	2drms/rms2d	Calculates pairwise RMSD between all frames of a trajectory.	method|measure	1
100	Atomic Correlation	atomiccorr	Calculates the correlation of atomic motions.	method|measure	5
101	Secondary Structure Assignment (DSSP)	dssp/secstruct	Assigns secondary structure elements (helix, sheet) to proteins.	method|algorithm	1
102	AKMA Units	AKMA system of units	A system of units (Angstrom, Kcal/mol, Mass, charge).	unit	1
103	Angstrom	Angstrom	A unit of length equal to 10^{-10} meters.	unit	4
104	Atomic Mass Unit	AMU	A unit of mass for expressing atomic and molecular weights.	unit	3
105	Elementary Charge	electron	The fundamental unit of electric charge.	unit	9
106	Atom Mask Selection	Atom Mask Selection Syntax	A syntax for specifying subsets of atoms, residues, or molecules.	method|identifier	2
107	Residue	residue	A single monomeric unit within a polymer, like an amino acid.	chemical entity	245
108	Molecule	molecule	An electrically neutral group of two or more atoms held together.	chemical entity	92
109	Distance-based Mask	Distance-based Masks	A selection syntax based on distance from another group of atoms.	method|identifier	8
110	File Tagging	Parameter/Reference Tagging	Assigning a short alias or nickname to a file.	identifier|method	1
111	Script Variable	script variables	User-defined variables for use within a cpptraj input script.	identifier	16
112	Data Set	data sets	Data generated by actions/analyses and stored internally.	data source	537
113	Data File	Data files	Files created by commands to store output data.	data format	54
114	Standard Data Format	Standard	The default, column-based data output format in cpptraj.	data format	934

115	Gnuplot Format	.gnu	A data file format for the Gnuplot plotting program.	data format	6
116	Xplor Grid Format	.xplor, .grid	A format for representing 3D grid data, from XPLOR-NIH.	data format	1
117	OpenDX Format	.dx	A format for 3D grid data for the OpenDX visualization program.	data format	9
118	Amber Replica Exchange Log	Amber REM log	Log file from an Amber Replica Exchange MD simulation.	data format|data source	2
119	Amber MD Output	Amber MDOUT	Standard output file from an Amber MD simulation containing energies.	data format|data source	2
120	Amber Eigenvector File	Amber Evecs	File format for storing eigenvectors from principal component analysis.	data format	1
121	Amber Constant pH Output	Amber Constant pH output	Output file from a constant pH molecular dynamics simulation.	data format|data source	1
122	CCP4 Map Format	.ccp4	A file format for electron density and other crystallographic maps.	data format	1
123	Pairwise Distance Cache	Pairwise Cache	A binary file storing pre-calculated pairwise distances for clustering.	data format|data source	5
124	Amber Prep File	Amber Prep File	An Amber file format defining a new residue or molecule.	data format	1
125	Amber OFF Library File	Amber OFF Library File	An Amber file format containing parameters for molecular fragments.	data format	2
126	Data Set Mathematics	Data Set Math	Performing mathematical operations directly on cpptraj data sets.	method	1
127	Coordinates Data Set	COORDS data set	A specialized data set for storing trajectory coordinate frames in memory.	data source|data format	37
128	Trajectory Data Set	TRAJ data set	A coordinate data set where frames are stored on disk.	data source|data format	5
129	Load Coordinates Command	loadcrd	Command to load a trajectory into an in-memory COORDS data set.	method	17
130	Create Coordinates Action	createcrd	An action to create a COORDS data set during trajectory processing.	method|process	10
131	Coordinates Action Command	crdaction	Command to perform a standard action on a COORDS data set.	method	15
132	Coordinates Output Command	crdout	Command to write a COORDS data set to a trajectory file.	method	11
133	Atomic Fluctuation	atomicfluct	Calculates the positional fluctuations of atoms, often as B-factors.	measure|method	12
134	Energy Minimization	emin	A process to find the nearest local energy minimum conformation.	process|method|algorithm	6
135	Steepest Descent Minimization	steepest descent minimization	An optimization algorithm that follows the negative gradient of the potential.	algorithm|method	1
136	Prepare for LEaP	prepareforleap	Command to process a structure (e.g., PDB) for Amber's LEaP program.	process|method	4
137	LEaP	LEaP	An Amber program for creating and editing molecular systems.	software	18
138	Disulfide Bond	disulfide	A covalent bond derived from two thiol groups.	chemical entity	10
139	Histidine	Histidine	An amino acid whose protonation state is often pH-dependent.	chemical entity	8
140	GLYCAM Force Field	GLYCAM	A force field specifically parameterized for carbohydrates.	model	9
141	Z-matrix	zmatrix	A representation of molecular conformation using internal coordinates.	model|data format	19

142	Data Set Selection	selectds	Prints the results of a data set selection expression.	method|identifier	8
143	Silence Actions	silenceactions	Prevents Actions from writing information to standard output.	method|state	1
144	Sort Ensemble Data	sortensembledata	Sorts data sets using replica information, like from constant pH.	method|process	5
145	Disk Cache	usediskcache	Controls the caching of data sets to disk to save memory.	method|state	3
146	Write Data	write | writedata	Immediately writes specified data sets to a file.	method|process	11
147	Active Reference	activeref	Sets the active reference structure for distance-based masks.	method|state	7
148	Calculate Expression	calc	Evaluates a given mathematical expression with formatting options.	method	9
149	Clear State	clear	Clears various lists of objects from the cpptraj state.	method|process	8
150	Create Data File	create	Adds specified data sets to a data file for later writing.	method	67
151	Create Data Set	createset	Generates a data set from a simple mathematical expression.	method	6
152	Data File Command	datafile	Passes formatting or other arguments to a specified data file.	method	40
153	Data Filter	datafilter	Filters data sets based on minimum and maximum value criteria.	method|process	7
154	Data Set Command	dataset	A command to manipulate data sets in various ways.	method	99
155	Nucleic Acid Torsion Angle	alpha|beta|gamma|delta|epsilon|zeta|chin	Backbone dihedral angles specific to nucleic acids.	measure|chemical entity	0
156	Protein Backbone Torsion Angle	phi|psi|omega	Backbone dihedral angles that determine protein secondary structure.	measure|chemical entity	1
157	Protein Side-chain Torsion Angle	chip	Side-chain dihedral angles in proteins.	measure|chemical entity	10
158	Distance Matrix	distance matrix	A 2D data set containing pairwise distances between particles.	data format|measure	8
159	Mass-Weighted Covariance Matrix	mass-weighted covariance	A covariance matrix where atomic motions are weighted by mass.	measure|data format	10
160	Distance Covariance Matrix	distance covariance	A matrix representing the covariance of inter-atomic distance fluctuations.	measure|data format	5
161	Debug Level	debug | prnlev	Sets the verbosity level for printing internal program information.	state	5
162	Ensemble Extension	ensextension	Toggles the automatic appending of ensemble member numbers to filenames.	method|state	5
163	Flatten Matrix	flatten	Converts a 2D matrix into a 1D array by summing or averaging.	method|algorithm	6
164	Marsaglia RNG	marsaglia	A specific type of random number generator.	algorithm	4
165	Mersenne Twister	mt	A widely used pseudo-random number generator algorithm.	algorithm	4
166	Permuted Congruential Generator	pcg32	A modern, high-quality pseudo-random number generator.	algorithm	4
167	Xoshiro128++ RNG	xo128	A fast, high-quality pseudo-random number generator.	algorithm	4
168	Read Data	readdata	Reads data from a file and stores it in cpptraj data sets.	method	46
169	Read Ensemble Data	readensembledata	Reads a series of data files as an ensemble for parallel processing.	method	7
170	Run Analysis	runanalysis	Immediately executes a specified analysis command or all queued analyses.	process	20
171	Atom Selection	select	Prints the atom numbers resulting from a mask expression.	method|identifier	31

172	System Command	System Commands	Commands that call external programs like 'ls' or 'gnuplot'.	software|method	3
173	Amber Topology File	.parm7	Amber's standard file for molecular topology and parameters.	data format	2
174	PDB (Protein Data Bank) File	.pdb	A standard text file format for 3D molecular structures.	data format	2
175	Mol2 File	.mol2	A molecular file format from Tripos for structure and properties.	data format	6
176	CIF (Crystallographic Information File)	.cif	A standard file format for crystallographic data.	data format	2
177	CHARMM PSF File	.psf	A protein structure file containing topology information for CHARMM.	data format	1
178	GROMACS Topology File	.top	A topology file for the GROMACS simulation package.	data format	1
179	SDF (Structure-Data File)	.sdf	A chemical file format for storing one or more molecules.	data format	2
180	Tinker ARC File	.arc	A trajectory or coordinate file format from the TINKER package.	data format	2
181	Angle Information	angleinfo | angles | printangles	Prints detailed information about angles in the topology.	method	2
182	Atom Information	atominfo | atoms | printatoms	Prints detailed information for selected atoms in the topology.	method	2
183	Generalized Born Radius	GBradius	An effective atomic radius used in Generalized Born implicit solvent models.	measure|model	3
184	Lennard-Jones Parameters	rVDW, eVDW	Parameters defining the van der Waals interactions between atoms.	model|measure	1
185	Bond Information	bondinfo | bonds | printbonds	Prints detailed information about bonds in the topology.	method	7
186	Change Topology	change	A command to modify various aspects of a topology.	method	51
187	Chain ID	chainid	An identifier used in PDB files to distinguish different polymer chains.	identifier	14
188	Original Residue Number	oresnums	The residue number as it appeared in the original input (e.g., PDB) file.	identifier	6
189	Insertion Code	icodes	A character used in PDB files to handle insertions in a sequence.	identifier	1
190	Compare Topologies	comparetop	Compares two topologies and reports differences in parameters and properties.	method	3
191	Hydrogen Mass Repartitioning	hmassrepartition	Increases hydrogen mass to allow for longer simulation time steps.	method|process	6
192	Improper Dihedral Information	improperinfo | impropers | printimpropers	Prints detailed information about improper dihedral angles.	method	1
193	Modify Box Parameters	parmbox	Modifies the periodic box dimensions and angles in a topology.	method	5
194	Truncated Octahedron	truncoct	A space-filling polyhedron used as a periodic boundary condition shape.	model|state	17
195	Strip from Topology	parmstrip	Permanently removes selected atoms from a topology in memory.	method|process	6
196	Write Topology	parmwrite	Writes a topology from memory to a file in a specified format.	method	10
197	Urey-Bradley Term	Urey-Bradley	A force field term describing interactions between 1,3-bonded atoms.	model	2
198	Scale Dihedral Force Constant	scaledihedralk	Scales the force constants of selected dihedral angles.	method	3
199	Define Solvent	solvent	Specifies which molecules in the topology should be treated as solvent.	method|state	131
200	Update Parameters	updateparameters	Updates parameters in a topology using values from another source.	method|process	5

201	Amber Trajectory Format	.crd	Amber's standard ASCII coordinate trajectory file format.	data format	1
202	Amber NetCDF Trajectory Format	.nc	Amber's binary trajectory format using the NetCDF library.	data format	6
203	Amber Restart File	.rst7, .rst	An Amber file containing coordinates and velocities for restarting simulations.	data format|data source	1
204	Amber NetCDF Restart File	.ncrst	A NetCDF-based restart file for Amber simulations.	data format|data source	1
205	CHARMM Coordinate File	.cor	A CHARMM file format for storing a single set of coordinates.	data format	1
206	Scripps Binpos Format	.binpos	A binary coordinate file format.	data format	1
207	GROMACS TRR File	.trr	A GROMACS trajectory file storing coordinates, velocities, and forces.	data format	1
208	GROMACS GRO File	.gro	A GROMACS coordinate file format for a single structure.	data format	1
209	GROMACS XTC File	.xtc	A compressed trajectory format from GROMACS for coordinates only.	data format	1
210	GROMACS TNG File	.tng	The next-generation, flexible trajectory format for GROMACS.	data format	1
211	SQM Input File	.sqm	An input file format for the semi-empirical QM program SQM.	data format	1
212	Desmond DTR File	.dtr	A trajectory file format used by the Desmond simulation software.	data format	1
213	LMOD Conflib File	.conflib	A conformational library file format for the LMOD software.	data format	1
214	MDTraj H5 File	.h5	An HDF5-based trajectory file format used by the MDTraj library.	data format	1
215	MDAnalysis H5MD File	.h5md	An HDF5-based trajectory file format used by the MDAnalysis library.	data format	1
216	Ensemble Size	ensemblesize	Specifies the number of trajectories in an ensemble for MPI efficiency.	method|state	9
217	Input Trajectory	trajin	Specifies an input trajectory file to be processed.	method|data source	99
218	Replica-Exchange Trajectory	remdtraj	Option to process trajectories from a replica-exchange simulation.	method|data source	12
219	Output Trajectory	trajout	Specifies an output trajectory file to be written.	method	71
220	PQR Format	dumpq | parse | vdw	A PDB-like format with atomic charges and radii in B-factor/occupancy columns.	data format	4
221	Anisotropic B-factor	adpdata	Describes atomic thermal motion anisotropically using a tensor.	measure|model	3
222	SYBYL Atom Type	sybyltype	Atom types defined in the SYBYL/Tripos force field.	model|identifier	3
223	XYZ File Format	.xyz	A simple text-based chemical file format for coordinates.	data format	1
224	Root-Mean-Square Fluctuation	rmsf	Calculates the root mean square fluctuation of specified atoms.	measure|method	8
225	Atom Mapping	atommap	Maps atoms between structures with different ordering or names.	method|process|algorithm	7
226	Automatic Imaging	autoimage	Automatically centers and images coordinates based on periodic boundaries.	method|process|algorithm	12
227	Average Structure	average	Calculates the mean coordinates of a set of frames.	method|process	191
228	Average Unit Cell	avgbox	Calculates the average unit cell vectors over a trajectory.	measure|method	17
229	Coordinate Bounds	bounds	Calculates the minimum and maximum coordinates for selected atoms.	measure|method	27

230	Periodic Box Manipulation	box	Sets or modifies the periodic box information for frames.	method|state	115
231	Centering	center	Translates coordinates to center a selection at a specific point.	method|process	1356
232	Structure Checking	check | checkoverlap | checkstructure	Checks for steric clashes or unusual bond lengths in frames.	method|process	1
233	Chirality	checkchirality	Determines the chirality (L or D) of amino acid alpha-carbons.	measure|chemical entity	9
234	Closest Solvent Molecules	closest | closestwaters	Retains a specified number of solvent molecules nearest to a solute.	method|process	3
235	Dihedral Clustering	clusterdihedral	Clusters trajectory frames based on dihedral angle values.	method|algorithm	6
236	Native Contacts	contacts	Calculates intermolecular or intramolecular contacts present in a reference structure.	measure|method	89
237	Reservoir-REMD	createreservoir	Creates a structure reservoir for use in reservoir REMD simulations.	method|process	4
238	Density Profile	density	Calculates number, mass, or charge density along an axis.	measure|method	172
239	Translational Diffusion	diffusion	Calculates the translational diffusion coefficient from mean-square displacement.	measure|method	87
240	Dihedral Angle	dihedral	Calculates the torsion angle defined by four atoms.	measure	135
241	Dihedral RMSD	dihrms | dihedralrms	Calculates the RMSD of dihedral angles relative to a reference.	measure|method	0
242	Energy Decomposition	enedecomp	Performs a per-atom decomposition of the potential energy.	method|process	5
243	SANDER API	esander	Calculates energies by interfacing with the Amber SANDER library.	method|software	8
244	Frame Filtering	filter	Selects frames for subsequent analysis based on data criteria.	method|process	22
245	Atom Order Fixing	fixatomorder	Reorders atoms to ensure molecules are defined by sequential atoms.	method|process	4
246	Image Bond Fixing	fiximagedbonds	Corrects covalent bonds that are broken by periodic imaging.	method|process	3
247	Voxel	voxel	A single grid point or box in a 3D grid analysis.	identifier	59
248	Deuterium Order Parameter	SCD	A measure of the orientational order of C-H bonds in lipids.	measure	13
249	Minimum/Maximum Distance	mindist/maxdist	Calculates the minimum or maximum distance between two groups of atoms.	measure|method	2
250	Minimum Image Distance	minimage	Calculates the shortest distance between atoms considering periodic boundaries.	measure|method	7
251	Ewald Summation	ewald	A method for calculating long-range electrostatic interactions in periodic systems.	method|algorithm	22
252	Particle Mesh Ewald (PME)	pme	An efficient implementation of the Ewald sum using Fast Fourier Transforms.	method|algorithm	24
253	Lennard-Jones PME	ljpme	An adaptation of the PME method for long-range Lennard-Jones interactions.	method|algorithm	4
254	Water Order Parameter	doorder	Calculates the tetrahedral order parameter for water molecules.	measure|method	8
255	Reference Water Density	refdens	The bulk density of water used as a reference in GIST calculations.	measure|unit	3
256	Oxygen Number Density	g_O	The number density of water oxygen atoms, normalized by bulk density.	measure	4
257	Hydrogen Number Density	g_H	The number density of water hydrogen atoms, normalized by bulk density.	measure	4
258	Translational Entropy	dTStrans	The contribution of translational motion to the total entropy.	measure	17
259	Orientational Entropy	dTSorient	The contribution of rotational motion to the total entropy.	measure	14
260	Solute-Water Interaction Energy	Esw	The interaction energy between the solute and surrounding water molecules.	measure	12

261	Water-Water Interaction Energy	Eww	The interaction energy between water molecules.	measure	20
262	Solute-Solvent Interaction Energy Density (per species)	Esw_mol_NAME-dens	Mean solute-solvent energy density for a specific solvent species.	measure|identifier	1
263	Solvent-Solvent Interaction Energy Density (per species)	Eww_mol_NAME-dens	Mean solvent-solvent energy density for a specific solvent species.	measure|identifier	1
264	Normalized PME Solvent Energy	PME-norm	Mean PME solvent energy per water molecule in a voxel.	measure|identifier	1
265	PME Solvent Energy Density	PME-dens	Mean PME solvent energy density in a voxel.	measure|identifier	3
266	Normalized Water-Water Interaction Energy	Eww-norm	Mean water-water interaction energy per water molecule in a voxel.	measure|identifier	6
267	Dipole Moment Density (X-component)	Dipole_x-dens	The x-component of the mean water dipole moment density.	measure|identifier	1
268	Dipole Moment Density (Y-component)	Dipole_y-dens	The y-component of the mean water dipole moment density.	measure|identifier	1
269	Dipole Moment Density (Z-component)	Dipole_z-dens	The z-component of the mean water dipole moment density.	measure|identifier	1
270	Dipole Moment Density Magnitude	Dipole-dens	The magnitude of the mean water dipole moment density (polarization).	measure|identifier	3
271	Neighbor Density	Neighbor-dens	The density of neighboring water molecules around a central water.	measure|identifier	1
272	Normalized Neighbor Count	Neighbor-norm	The mean number of neighbors per water molecule in a voxel.	measure|identifier	3
273	Normalized Tetrahedral Order Parameter	Order-norm	The average tetrahedral order parameter for water molecules in a voxel.	measure|identifier	4
274	Tetrahedral Order Parameter	q_tet	A measure of the tetrahedral arrangement of a water molecule's neighbors.	measure|model	3
275	Placevent	Placevent	A program to define spherical hydration sites from density distributions.	software	1
276	Inhomogeneous Fluid Solvation Theory	Inhomogeneous fluid solvation theory	The theoretical framework underlying the GIST analysis method.	model|method	2
277	TIP3P Water Model	TIP3P	A specific three-site rigid water model.	model|chemical entity	3
278	TIP4PEW Water Model	TIP4PEW	A specific four-site rigid water model optimized for Ewald sums.	model|chemical entity	1
279	TIP4P Water Model	TIP4P	A specific four-site rigid water model.	model|chemical entity	1
280	TIP5P Water Model	TIP5P	A specific five-site rigid water model.	model|chemical entity	1
281	Tip3PFW Water Model	Tip3PFW	A flexible three-site water model.	model|chemical entity	1

282	SPCE Water Model	SPCE	A standard three-site rigid water model (Simple Point Charge/Extended).	model|chemical entity	1
283	SPCFW Water Model	SPCFW	A flexible three-site water model.	model|chemical entity	1
284	Solvent Bridge	bridging	A solvent molecule that is hydrogen-bonded to two or more solute residues.	chemical entity|state	14
285	Karplus Equation	Karplus parameters	An equation that relates dihedral angles to J-coupling constants.	model|method	3
286	Atom Keeping	keep	An action that retains only a specified subset of atoms.	method|process	43
287	Lipid SCD Order Parameter Calculation	lipidscd	An action to calculate lipid order parameters |SCD| for acyl chains.	method|measure	4
288	Multiple Dihedral Calculation	multidihedral	An action to calculate multiple dihedral angles of specified types.	method|process	11
289	Multiple Ring Pucker Calculation	multipucker	An action to calculate ring pucker for multiple residues.	method|process	4
290	Altona & Sundaralingam Pucker	altona	A method for describing the conformation of five-membered rings.	method|algorithm	14
291	Cremer & Pople Pucker	cremer	A method for describing the conformation of cyclic molecules.	method|algorithm	16
292	Multiple Vector Calculation	multivector	An action to calculate multiple vectors between specified atom pairs.	method|process	4
293	3DNA	3dna	A reference software package for nucleic acid structure analysis.	software|method	10
294	Base Pair Parameter	shear|stretch|stagger|buckle|prop|open	A parameter describing the geometry and orientation of a base pair.	measure|identifier	0
295	Base Pair Step Parameter	shift|slide|rise|title|roll|twist	A parameter describing the geometry between two consecutive base pairs.	measure|identifier	0
296	Helical Parameter	xdisp|ydisp|hrise|incl|tip|htwist	A parameter describing the global helical structure of a nucleic acid.	measure|identifier	0
297	Native Contact Analysis	nativecontacts	An action to identify and track contacts present in a reference structure.	method|analysis	8
298	Atom Remapping	remap	An action to reorder atoms according to a provided mapping.	method|process	6
299	Coordinate Rotation	rotate	An action to rotate coordinates around a specified axis or by a matrix.	method|process	38
300	secstruct	secstruct	A command to calculate secondary structure propensities using DSSP.	method|analysis	12
301	DSSP	DSSP	A method for assigning secondary structure based on hydrogen bonds.	algorithm|method	12
302	Kabsch and Sander	Kabsch and Sander	The authors of the DSSP secondary structure assignment method.	data source	2
303	ptrajformat	ptrajformat	An output format for secondary structure similar to ptraj software.	data format	6
304	betadetail	betadetail	An option to report detailed parallel and anti-parallel beta structures.	method|state	6
305	Parallel beta	Para	A secondary structure motif where beta strands run in parallel.	state|chemical entity	8
306	Anti-parallel beta	Anti	A secondary structure motif where beta strands run in opposite directions.	state|chemical entity	7
307	3-10 helix	3-10	A type of helical secondary structure with three residues per turn.	state|chemical entity	3

308	Alpha helix	Alpha	A common secondary structure motif in proteins.	state|chemical entity	27
309	Pi helix	Pi	A type of helical secondary structure with 4.4 residues per turn.	state|chemical entity	13
310	Turn	Turn	A secondary structure element that reverses the polypeptide chain direction.	state|chemical entity	18
311	Bend	Bend	A region of a protein with high curvature.	state|chemical entity	3
312	Extended beta	E	A secondary structure of consecutive beta bridges of the same type.	state|chemical entity	219
313	beta Bridge	B	An isolated pair of residues in a beta-sheet conformation.	state|chemical entity	58
314	gnuplot	gnuplot	A command-line driven graphing utility for data visualization.	software	25
315	xmgrace	xmgrace	A 2D plotting tool for X Window System.	software	10
316	zeromomentum	zeromomentum	A process to ensure the total momentum of selected atoms is zero.	process|method	3
317	Å²	Å²	A unit of area, Angstroms squared.	unit	0
318	degrees of freedom	degrees of freedom	The number of independent ways a system can move.	measure|model	3
319	toroidal-view-preserving scheme	TOR	An algorithm for correcting box fluctuations in diffusion calculations.	algorithm|method	12
320	1x10?? cm²/s	1x10?? cm²/s	A common unit for reporting diffusion coefficients.	unit	0
321	translate	translate	A command to translate atoms by a specified vector.	process	11
322	periodic boundary conditions	periodic boundary conditions	A method to simulate a large system by replicating a unit cell.	model|method	8
323	dipole	dipole	A vector representing the separation of positive and negative charges.	measure|chemical entity	30
324	Debye	Debye	A unit of electric dipole moment.	unit	13
325	self-diffusion coefficient	D	A measure of the translational mobility of particles.	measure	48
326	Gaussian function	Gaussian	A function used to represent atomic density in volmap.	model|algorithm	11
327	van der Waals radius	vdw	A measure of the effective size of an atom.	measure|model	22
328	VMD	VMD	Visual Molecular Dynamics, a molecular visualization program.	software	6
329	cubic spline interpolation	splinedx	A method for interpolating data points smoothly.	algorithm|method	4
330	solvation shell	solvation shell	Layers of solvent molecules surrounding a solute.	model|chemical entity	0
331	space group	group	A description of the symmetry of a crystal structure.	model|identifier	37
332	autocorr	autocorr	An analysis command to calculate autocorrelation for data sets.	analysis|method	3
333	auto-covariance	nocovar	A measure of the covariance of a signal with itself at different time lags.	measure	5
334	Fast Fourier Transform	FFT	An algorithm to compute the discrete Fourier transform and its inverse.	algorithm	14
335	avg	avg	An analysis command to calculate average and other statistics for data sets.	analysis|method	50

336	standard deviation	sd	A measure of the amount of variation or dispersion of a set of values.	measure	34
337	calcdiffusion	calcdiffusion	An analysis command to calculate diffusion from multiple time origins.	analysis|method	12
338	calcstate	calcstate	An analysis command to define and analyze conformational states from data.	analysis|method	7
339	cluster	cluster	An analysis command to perform cluster analysis on frames or data.	analysis|method	141
340	hierarchical agglomerative clustering	hieragglo	A bottom-up clustering method where each observation starts in its own cluster.	algorithm	4
341	DBSCAN	dbscan	A density-based clustering algorithm that groups together points that are closely packed.	algorithm	15
342	k-means clustering	kmeans	A method of vector quantization that aims to partition n observations into k clusters.	algorithm	5
343	density peaks clustering	dpeaks	A clustering method based on identifying cluster centers as high-density peaks.	algorithm	9
344	Euclidean distance	euclid	The straight-line distance between two points in Euclidean space.	measure	3
345	Manhattan distance	manhattan	A distance metric calculated as the sum of the absolute differences of coordinates.	measure	3
346	sieve	sieve	A technique in clustering to reduce computation by using a subset of frames.	method|process	13
347	Davies-Bouldin Index	DBI	A metric for evaluating the quality of a clustering algorithm's output.	measure	10
348	pseudo-F statistic	pSF	A metric for determining the number of clusters in a data set.	measure	13
349	SSR/SST	SSRSST	The ratio of sum of squares regression to total sum of squares, a clustering metric.	measure	8
350	cluster silhouette	sil	A measure of how similar an object is to its own cluster compared to others.	measure	9
351	K-dist plot	kdist	A plot used to help determine the epsilon parameter for DBSCAN.	analysis|method	15
352	Pearson product-moment correlation coefficient	crosscorr	A measure of the linear correlation between two sets of data.	measure	3
353	crankshaft motion	crank	A type of localized conformational transition in a polymer chain.	state|process	5
354	curvefit	curvefit	An analysis command for non-linear curve fitting of data sets.	analysis|method	6
355	Levenberg-Marquardt algorithm	Levenberg-Marquardt	An iterative algorithm used to solve non-linear least squares problems.	algorithm	0
356	diagmatrix	diagmatrix	An analysis command to diagonalize a matrix, yielding eigenvalues and eigenvectors.	analysis|method	16
357	Principal Component Analysis	PCA	A statistical method to convert observations into linearly uncorrelated principal components.	method|analysis	11
358	Quasiharmonic Analysis	thermo	A method to calculate thermodynamic properties from vibrational frequencies.	method|analysis	9
359	NMWiz	nmwiz	A VMD plugin for visualizing and analyzing normal modes.	software	5
360	cm?^{1}	cm?^{1}	Wavenumber, a unit of frequency often used in spectroscopy.	unit	0
361	evalplateau	evalplateau	An analysis command to evaluate if a data set has reached a plateau.	analysis|method	3
362	Hausdorff distance	hausdorff	A measure of how far two subsets of a metric space are from each other.	measure|analysis	22
363	parallelanalysis	parallelanalysis	A command to run multiple analyses in parallel using MPI.	process|software	6
364	histogram	hist	A command to create an N-dimensional histogram from data sets.	method|analysis	31
365	free energy	free	An estimation of free energy from bin populations via Boltzmann inversion.	measure|method	14
366	Boltzmann's constant	k_B	A physical constant relating temperature to kinetic energy of particles.	measure|data source	1

367	AMD boost energy	amd	Energy values from Accelerated Molecular Dynamics used for reweighting.	measure|data source	6
368	pseudo-trajectory	traj3d	A trajectory-like file generated from 3D histogram data for visualization.	data format	12
369	Lamor frequency	freq	The precession frequency of a magnetic moment in a magnetic field.	measure|unit	5
370	MHz	MHz	Megahertz, a unit of frequency (10^6 Hz).	unit	3
371	T1 relaxation	T1	The longitudinal or spin-lattice relaxation time in NMR.	measure	9
372	T2 relaxation	T2	The transverse or spin-spin relaxation time in NMR.	measure	3
373	Legendre polynomials	order	A system of complete and orthogonal polynomials used in time correlation.	model|algorithm	158
374	S2 order parameter	orderparamfile	A measure of the motional restriction of a bond vector in NMR.	measure	2
375	correlation time	tcorr	The time scale over which a system's properties remain correlated.	measure	14
376	nanosecond	ns	A unit of time equal to 10?? seconds.	unit	11
377	bandwidth	bandwidth	A smoothing parameter that controls the trade-off in KDE.	measure	4
378	lifetime	lifetime	A command to analyze the duration of specific states or interactions.	method|analysis	69
379	lowestcurve	lowestcurve	A command to generate a curve by averaging the lowest points in bins.	method|analysis	3
380	RMS fluctuations	fluct	Root-mean-square fluctuations of atomic positions, calculated from modes.	measure	13
381	root-mean-square inner product	rmsip	A measure of the overlap or similarity between two sets of modes.	measure|analysis	5
382	Bose statistics	bose	Quantum statistics used to populate vibrational modes at low temperatures.	model	3
383	principal component	pcmin	A vector representing a direction of maximum variance in a dataset.	measure|model	15
384	multicurve	multicurve	A command to perform non-linear curve fitting for multiple data sets simultaneously.	method|analysis	3
385	multi-exponential function	mexp	A function composed of a sum of several exponential terms.	model	4
386	multihist	multihist	A command to generate multiple 1D histograms from various data sets.	method|analysis	3
387	phipsi	phipsi	A command to analyze and plot average phi and psi dihedral angles.	method|analysis	11
388	phi dihedral	phi	A protein backbone dihedral angle (C-N-CA-C).	measure|chemical entity	51
389	psi dihedral	psi	A protein backbone dihedral angle (N-CA-C-N).	measure|chemical entity	48
390	projectdata	projectdata	A command to project 1D data sets onto previously generated eigenmodes.	method|analysis	6
391	remlog	remlog	A command to analyze log files from Replica Exchange Molecular Dynamics (REMD).	method|analysis	19
392	Replica Exchange Molecular Dynamics	REMD	An enhanced sampling method that simulates multiple replicas at different temperatures.	method|process	33
393	round-trip time	stats	In REMD, the time for a replica to travel across the entire temperature range and back.	measure	8
394	2D RMSD	rms2d	A matrix of RMSD values comparing every frame in a trajectory to every other frame.	measure|analysis	14
395	RMS average correlation	rmsavgcorr	The average RMSD of running-averaged coordinates over increasing time windows.	measure|analysis	15
396	downhill simplex minimizer	amoeba	An optimization algorithm for finding the minimum of a function in a multidimensional space.	algorithm	2

397	finite difference	slope	A mathematical expression that approximates a derivative.	algorithm|measure	18
398	cubic spline	spline	A piecewise polynomial function used for interpolation of data points.	algorithm|model	10
399	NOE violation	noeout	An instance where a simulated distance falls outside the bounds of an NOE restraint.	measure|state	4
400	<r??>?¹/? averaged distance	R6	A specific form of distance averaging used in NMR structure calculation.	measure	5
401	Gaussian quadrature	nq	A numerical method for approximating the definite integral of a function.	algorithm	8
402	bootstrap analysis	bs_samples	A resampling statistical method used for estimating distributions and errors.	method|analysis	4
403	Time-lagged Independent Component Analysis	tica	A method to find the slowest dynamical processes from molecular simulation data.	method|analysis	12
404	kinetic map	map kinetic	A transformation of TICA eigenvectors to approximate kinetic distances between states.	method|model	0
405	commute map	map commute	A transformation of TICA eigenvectors to approximate commute distances between states.	method|model	0
406	vectormath	vectormath	A command to perform mathematical operations like dot or cross products on vectors.	method|analysis	4
407	dot product	dotproduct	An operation that returns a scalar representing the projection of one vector onto another.	measure	7
408	cross product	crossproduct	A binary operation on two vectors that results in a third vector perpendicular to both.	measure	3
409	wavelet analysis	wavelet	A method that decomposes a time series into time and frequency components.	method|analysis	33
410	continuous wavelet transform	CWT	A transform that provides an overcomplete representation of a signal by letting the translation and scale parameters vary continuously.	algorithm|method	4
411	Morlet wavelet	morlet	A non-orthogonal complex wavelet used for time-frequency analysis.	model	7
412	Paul wavelet	paul	A type of complex-valued analytic wavelet.	model	5
413	Wavelet Analysis Feature Extraction	WAFEX	A method using clustering on wavelet maps to identify significant motions.	method|analysis	3
	Distance RMSD	drms | drmsd	Calculates the RMSD of internal pairwise distances.	measure|method	4
	IDEA Matrix	IDEA	A matrix from the Isotropically Distributed Ensemble of Affine-rigid-body-motions analysis.	measure|data format	18
	LCPO (Linear Combination of Pairwise Overlaps)	LCPO	An algorithm for calculating solvent accessible surface area.	algorithm	2
	Running Average	runavg | runningaverage	Calculates a running average of coordinates over a time window.	method|process	12
	thermodynamic integration	ti	A method for calculating free energy differences by integrating along a path.	method|analysis	22
	Bond Parameter Information	bondparminfo	Prints the table of unique bond parameters from the topology.	method	3
	Dihedral Information	dihedralinfo | dihedrals | printdihedrals	Prints detailed information about dihedral angles in the topology.	method	2
	Molecule Information	molinfo	Prints information about the molecules defined in the topology.	method	8
	Topology Information	parminfo	Prints a summary of the information contained in a topology file.	method	6
	Urey-Bradley Information	printub | ubinfo	Prints information about Urey-Bradley 1-3 interaction terms.	method	1

	Residue Information	resinfo	Prints detailed information about residues in the topology.	method	5
	CHARMM Restart File	.res	A file for restarting a CHARMM simulation.	data format|data source	1
	LCPO algorithm	LCPO algorithm	An algorithm for calculating solvent accessible surface area.	algorithm|method	1